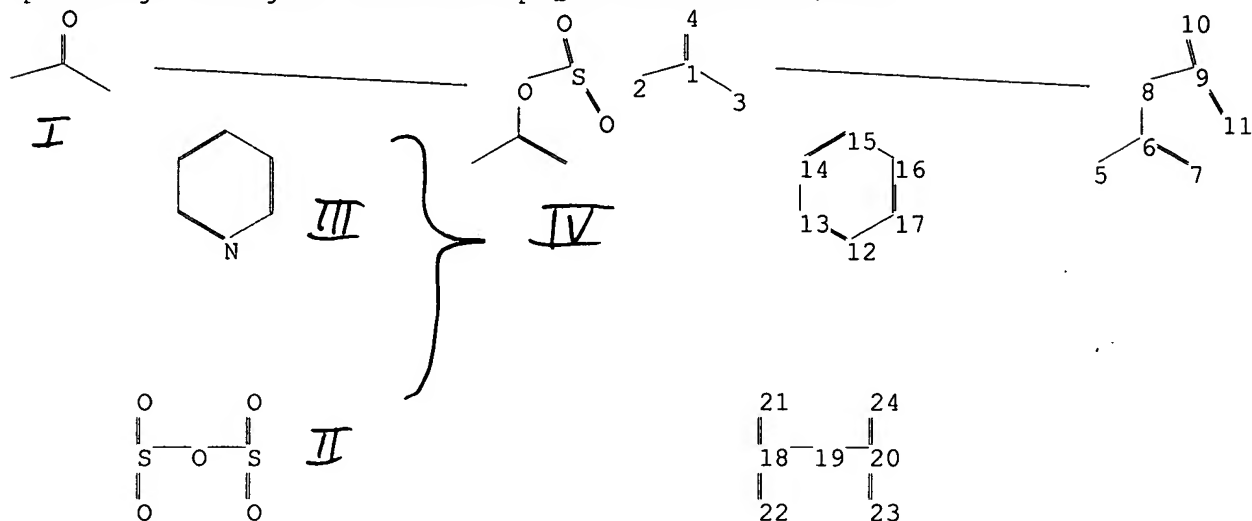


identification.

=>

Uploading C:\Program Files\Stnexp\Queries\10518492\1.str



chain nodes :

1 2 3 4 5 6 7 8 9 10 11 18 19 20 21 22 23 24

ring nodes :

12 13 14 15 16 17

chain bonds :

1-2 1-3 1-4 5-6 6-7 6-8 8-9 9-10 9-11 18-19 18-21 18-22 19-20 20-23
20-24

ring bonds :

12-13 12-17 13-14 14-15 15-16 16-17

exact/norm bonds :

1-4 6-8 8-9 9-10 9-11 18-19 18-21 18-22 19-20 20-23 20-24

exact bonds :

1-2 1-3 5-6 6-7

normalized bonds :

12-13 12-17 13-14 14-15 15-16 16-17

Match level :

1:CLASS 2:CLASS 3:CLASS 4:CLASS 5:CLASS 6:CLASS 7:CLASS 8:CLASS 9:CLASS

10:CLASS 11:CLASS 12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:Atom 18:CLASS

19:CLASS 20:CLASS 21:CLASS 22:CLASS 23:CLASS 24:CLASS

fragments assigned product role:

containing 5

fragments assigned reactant/reagent role:

containing 1

containing 12

containing 18
node mappings:
1:6 4:8 2:5 3:7

L1 STRUCTURE UPLOADED

=> d
L1 HAS NO ANSWERS
L1 STR

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

Structure attributes must be viewed using STN Express query preparation.

=> d
L1 HAS NO ANSWERS
L1 STR

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

Structure attributes must be viewed using STN Express query preparation.

=> s l1 full
FULL SEARCH INITIATED 13:03:26 FILE 'CASREACT'
SCREENING COMPLETE - 278 REACTIONS TO VERIFY FROM

52 DOCUMENTS

100.0% DONE 278 VERIFIED 22 HIT RXNS
SEARCH TIME: 00.00.01

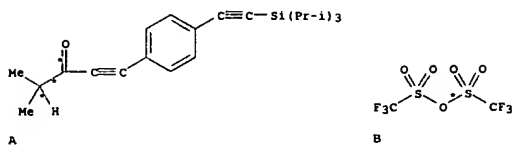
9 DOCS

L2 9 SEA SSS FUL L1 (22 REACTIONS)

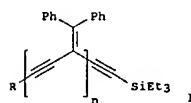
=> d ibib abs hit 1-9

L2 ANSWER 1 OF 9 CASREACT COPYRIGHT 2006 ACS on STN
 ACCESSION NUMBER: 143:7446 CASREACT
 TITLE: Synthesis and characterization of cross-conjugated
 oligo(phenylene enynylene)s
 AUTHOR(S): Cho, Joon; Zhao, Yuming; Tykwinski, Rik R.
 CORPORATE SOURCE: Department of Chemistry, University of Alberta,
 Edmonton, AB, T6G 2G2, Can.
 SOURCE: ARKIVOC (Gainesville, FL, United States) (2005), (4),
 142-150
 CODEN: AGFUAR
 URL:
 http://www.arkat-usa.org/ark/journal/2005/I04_2ef
 irov/1369/1369.pdf
 PUBLISHER: Arkat USA Inc.
 DOCUMENT TYPE: Journal; (online computer file)
 LANGUAGE: English
 AB The synthesis and characterization of a series of cross-conjugated
 oligo(phenylene enynylene)s via the Sonogashira protocol is reported.
 The structural properties of these oligomers have been established by ¹H and
¹³C NMR and IR spectroscopies, as well as mass spectrometry. Their
 electronic absorption and emission behavior has been investigated via
 UV/Vis and fluorescence spectroscopy. The results of this study
 demonstrate that electronic communication along the conjugated framework
 of these oligomers is limited due to the presence of a cross-conjugated
 enyne framework and arylene fragments.
 REFERENCE COUNT: 20 THERE ARE 20 CITED REFERENCES AVAILABLE FOR
 THIS
 FORMAT RECORD. ALL CITATIONS AVAILABLE IN THE RE

RX(1) OF 28 ...A + B ==> C...

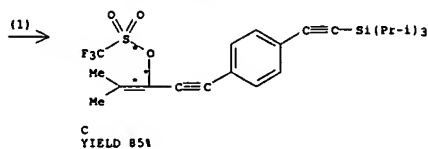


L2 ANSWER 2 OF 9 CASREACT COPYRIGHT 2006 ACS on STN
 ACCESSION NUMBER: 142:279793 CASREACT
 TITLE: Synthesis, structure, and nonlinear optical
 properties of cross-conjugated perphenylated
 iso-polydiacetylenes
 AUTHOR(S): Zhao, Yuming; Slepko, Aaron D.; Akoto, Clement Osei;
 McDonald, Robert; Hegmann, Frank A.; Tykwinski, Rik
 R.
 CORPORATE SOURCE: Department of Chemistry, Memorial University of
 Newfoundland, St. John's, NL, A1B 3X7, Can.
 SOURCE: Chemistry--A European Journal (2005), Volume Date
 2004, 11(1), 321-329
 CODEN: CEUJED; ISSN: 0947-6539
 WILEY-VCH Verlag GmbH & Co. KGaA
 PUBLISHER: Journal
 DOCUMENT TYPE: English
 LANGUAGE: English
 GI



AB Monodisperse, cross-conjugated perphenylated iso-polydiacetylene
 (iso-PDA)
 oligomers I (R = Me3Si, n = 1; R = Et3Si; n = 2, 3, 5, 7, 9, 11, 13, 15)
 have been synthesized by using a palladium-catalyzed cross-coupling
 protocol. Structural characteristics elucidated by x-ray crystallog.
 anal. demonstrate a non-planar backbone conformation for the oligomers
 due to the steric interactions between alkylidene Ph groups. The electronic
 absorption spectra of the oligomers show a slight red-shift of the
 maximum absorption wavelength as the chain length increases from dimer I (n = 2)
 to pentadecamer I (n = 15) a trend that has saturated by the stage of
 nonamer I (n = 9). Fluorescence spectroscopy confirms that the pendent Ph groups
 present on the oligomer framework enhance emission, and the relative
 emission intensity consistently increases as a function of chain length
 n.
 The mol. third-order nonlinearities, $\chi^{(3)}$, for this oligomer series
 have been measured via differential optical Kerr effect (DOKE) detection
 and show a superlinear increase as a function of the oligomer chain
 length
 n. Mol. modeling and spectroscopic studies suggest that iso-PDA
 oligomers
 I (n > 7) adopt a coiled, helical conformation in solution
 REFERENCE COUNT: 66 THERE ARE 66 CITED REFERENCES AVAILABLE FOR
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 FORMAT RECORD. ALL CITATIONS AVAILABLE IN THE RE

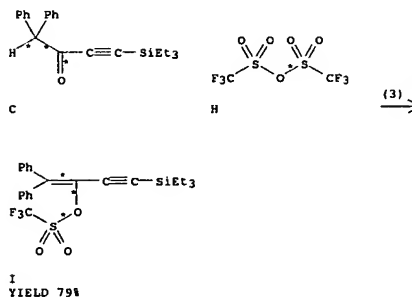
L2 ANSWER 1 OF 9 CASREACT COPYRIGHT 2006 ACS on STN (Continued)



RX(1)
 RCT A 852459-84-8, B 358-23-6
 RGT D 38222-83-2 Me-(t-Bu)2-pyridine
 PRO C 852459-83-7
 SOL 75-09-2 CH2Cl2
 CON SUBSTAGE(1) 0 deg C
 SUBSTAGE(2) 0 deg C -> room temperature
 SUBSTAGE(3) 4 hours, room temperature
 NTE Sonogashira coupling

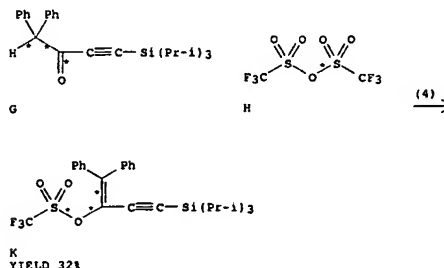
L2 ANSWER 2 OF 9 CASREACT COPYRIGHT 2006 ACS on STN (Continued)

RX(3) OF 125 ...C + H ==> I...



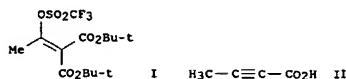
RX(3)
 RCT C 845725-73-7, H 358-23-6
 RGT J 505-48-8 2,6-Di-t-Bu-pyridine
 PRO I 339577-77-4
 SOL 75-09-2 CH2Cl2
 CON room temperature

RX(4) OF 125 ...G + H ==> K...



L2 ANSWER 2 OF 9 CASREACT COPYRIGHT 2006 ACS on STN (Continued)
 RX(4) RCT G 845725-74-8, H 358-23-6
 RGT J 585-48-8 2,6-Di-t-Bu-pyridine
 PRO K 845725-75-9
 SOL 75-09-2 CH2Cl2
 CON room temperature

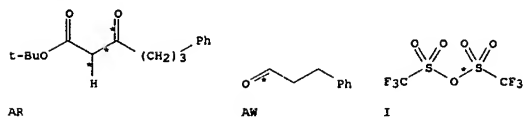
L2 ANSWER 3 OF 9 CASREACT COPYRIGHT 2006 ACS on STN
 ACCESSION NUMBER: 141:140115 CASREACT
 TITLE: Decarboxylative elimination of enol triflates as a general synthesis of acetylenes
 AUTHOR(S): Fleming, Ian; Ramarao, Chandrashekar
 CORPORATE SOURCE: Department of Chemistry, Cambridge, CB2 1EW, UK
 SOURCE: Organic & Biomolecular Chemistry (2004), 2(10), 1504-1510
 CODEN: OBCRAK; ISSN: 1477-0520
 PUBLISHER: Royal Society of Chemistry
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 GI



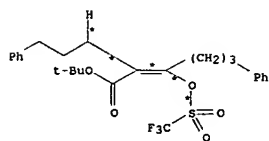
AB The enol trifluoromethanesulfonates of tert-Bu β -keto diesters and β -keto esters can be hydrolyzed to the corresponding carboxylic acids by dissoln. in trifluoroacetic acid. The dicarboxylic acids undergo mild decarboxylative elimination to give acetylenic acids in aqueous sodium bicarbonate solution at room temperature. Similarly, monocarboxylic acids give terminal and mid-chain acetylenes by refluxing in acetone with potassium carbonate. One of the substituents on the acetylenes can be Me, primary alkyl, secondary alkyl or ethynyl, and the other can be a carboxylic acid, hydrogen or primary alkyl, but the enol trifluoromethanesulfonates could not be prepared when one of the substituents was tert-Bu, nor when both substituents on the precursor to the acetylene were secondary alkyl. For example, reaction of trifluoromethanesulfonic acid anhydride with (acetyl)propanedioic acid bis(1,1-dimethylethyl) ester gave a desired enol triflate, [1-[(trifluoromethyl)sulfonyl]oxy]ethylidene]propanedioic acid bis(1,1-dimethylethyl) ester (I). Saponification of I gave the diacid, [1-[(trifluoromethyl)sulfonyl]oxy]ethylidene]propanedioic acid. Decarboxylation of the acid gave 2-butyric acid (II).
 REFERENCE COUNT: 46 THERE ARE 46 CITED REFERENCES AVAILABLE FOR THIS
 RECORD. ALL CITATIONS AVAILABLE IN THE RE
 FORMAT

RX(96) OF 118 COMPOSED OF RX(22), RX(26), RX(29)
 RX(96) AR + AW + I ==> BK

L2 ANSWER 3 OF 9 CASREACT COPYRIGHT 2006 ACS on STN (Continued)



3
 STEPS
 →



YIELD 86%

RX(22) RCT AR 235087-24-8, AW 104-53-0

STAGE(1)
 RGT AY 7550-45-0 TiCl4, AZ 110-86-1 Pyridine
 SOL 109-99-9 THF, 75-09-2 CH2Cl2
 CON SUBSTAGE(1) 30 minutes, 0 deg C
 SUBSTAGE(2) 16 hours, room temperature

STAGE(2)
 RGT F 12125-02-9 NH4Cl
 SOL 7732-18-5 Water
 CON room temperature

PRO AX 725340-58-9
 NTE stereoselective, isomer mix.

RX(26) RCT AX 725340-58-9
 RGT BF 1333-74-0 H2
 PRO BE 235087-25-9
 CAT 7440-05-3 Pd
 SOL 67-56-1 MeOH
 CON 24 hours, room temperature

RX(29) RCT BE 235087-25-9

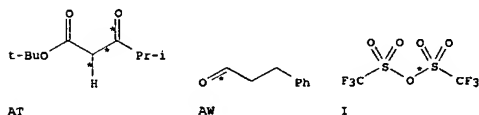
L2 ANSWER 3 OF 9 CASREACT COPYRIGHT 2006 ACS on STN (Continued)

STAGE(1)
 RGT L 7646-69-7 NaH
 SOL 60-29-7 Et2O
 CON 1 hour, 0 deg C
 STAGE(2)
 RCT I 358-23-6
 CON SUBSTAGE(1) 1 hour, 0 deg C
 SUBSTAGE(2) 1 hour, room temperature

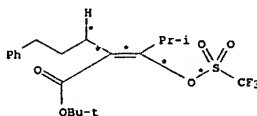
STAGE(3)
 RGT F 12125-02-9 NH4Cl
 SOL 7732-18-5 Water
 CON room temperature

PRO BK 235087-28-2

RX(98) OF 118 COMPOSED OF RX(23), RX(27), RX(30)
 RX(98) AT + AW + I ==> BL



3
 STEPS
 →



YIELD 92%

RX(23) RCT AT 94250-54-1, AW 104-53-0

STAGE(1)
 RGT AY 7550-45-0 TiCl4, AZ 110-86-1 Pyridine
 SOL 109-99-9 THF, 75-09-2 CH2Cl2
 CON SUBSTAGE(1) 30 minutes, 0 deg C
 SUBSTAGE(2) 16 hours, room temperature

STAGE(2)
 RGT F 12125-02-9 NH4Cl
 SOL 7732-18-5 Water
 CON room temperature

L2 ANSWER 3 OF 9 CASREACT COPYRIGHT 2006 ACS on STN (Continued)
 PRO BA 725340-63-6
 NTE stereoselective, isomer mix.

RX(27) RCT BA 725340-63-6
 RGT BF 1333-74-0 H2
 PRO BI 235087-26-0
 CAT 7440-05-3 Pd
 SOL 67-56-1 MeOH
 CON 24 hours, room temperature

RX(30) RCT BI 235087-26-0

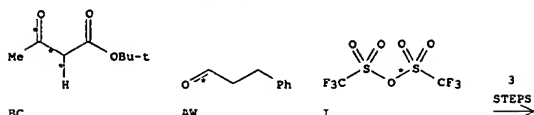
STAGE(1)
 RGT L 7646-69-7 NaH
 SOL 60-29-7 Et2O
 CON 1 hour, 0 deg C

STAGE(2)
 RCT I 358-23-6
 CON SUBSTAGE(1) 1 hour, 0 deg C
 SUBSTAGE(2) 1 hour, room temperature

STAGE(3)
 RGT F 12125-02-9 NH4Cl
 SOL 7732-18-5 Water
 CON room temperature

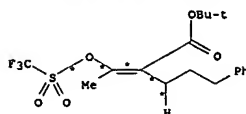
PRO BL 235087-30-6

RX(100) OF 118 COMPOSED OF RX(25), RX(28), RX(31)
 RX(100) BC + AW + I ==> BM



L2 ANSWER 3 OF 9 CASREACT COPYRIGHT 2006 ACS on STN (Continued)
 PRO BM 725340-88-5

L2 ANSWER 3 OF 9 CASREACT COPYRIGHT 2006 ACS on STN (Continued)



BM
 YIELD 71%

RX(25) RCT BC 1694-31-1, AW 104-53-0

STAGE(1)
 RGT AY 7550-45-0 TiCl4, AZ 110-86-1 Pyridine
 SOL 109-99-9 THF, 75-09-2 CH2Cl2
 CON SUBSTAGE(1) 30 minutes, 0 deg C
 SUBSTAGE(2) 16 hours, room temperature

STAGE(2)
 RGT F 12125-02-9 NH4Cl
 SOL 7732-18-5 Water
 CON room temperature

PRO BD 725340-53-4
 NTE stereoselective, isomer mix.

RX(28) RCT BD 725340-53-4
 RGT BF 1333-74-0 H2
 PRO BJ 725340-75-0
 CAT 7440-05-3 Pd
 SOL 67-56-1 MeOH
 CON 24 hours, room temperature

RX(31) RCT BJ 725340-75-0

STAGE(1)
 RGT L 7646-69-7 NaH
 SOL 60-29-7 Et2O
 CON 1 hour, 0 deg C

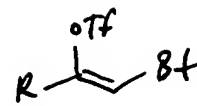
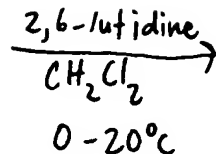
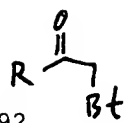
STAGE(2)
 RCT I 358-23-6
 CON SUBSTAGE(1) 1 hour, 0 deg C
 SUBSTAGE(2) 1 hour, room temperature

STAGE(3)
 RGT F 12125-02-9 NH4Cl
 SOL 7732-18-5 Water
 CON room temperature

L2 ANSWER 4 OF 9 CASREACT COPYRIGHT 2006 ACS on STN
 ACCESSION NUMBER: 140:111001 CASREACT
 TITLE: Fragmentations of (E)- and (Z)-isomers of 2-methylbuten-1-yl(aryl) iodonium triflates:
 competing mechanisms for enol triflate formation
 AUTHOR(S): Hinkle, Robert J.; Mikowski, Ann M.
 CORPORATE SOURCE: Dep. Chem., The College of William and Mary, Williamsburg, VA, 23187-8795, USA
 SOURCE: ARKIVOC (Gainesville, FL, United States) (2003), (6), 201-212
 CODEN: AGFUAR
 URL: <http://www.arkat-usa.org/ark/journal/2003/Varvogil>
 PUBLISHER: Arkat USA Inc.
 DOCUMENT TYPE: Journal; (online computer file)
 LANGUAGE: English
 AB We examined fragmentation reactions of (E)- and (Z)-2-methylbuten-1-yl(aryl)iodonium triflates (aryl = C6H5-, 4-(CF3)C6H4, 3,5-(CF3)2C6H4-) to afford aryl iodides and six enol triflates. Four of these vinyl triflates involve alkyl migrations followed by triflate trapping of secondary vinyl cations whereas two do not involve migrations. Fragmentation rates in dry, neutral CDCl3 were determined as were the distributions of enol triflate products. The ratios of rate consts. for the (E)-/(Z)- isomers ranged between 5.0 and 8.5 and, in all salts, the rearranged enol triflate derived from migration of the alkyl moiety trans- to the aryl-iodonio- nucleofuge was observed in the greatest quantities. These data indicate that the fragmentation rates are significantly determined by the migratory aptitude of the trans-β-alkyl substituent and departure of the aryl-iodonio-nucleofuge occurs by anchimeric assistance. The ratios of inverted "unrearranged" enol triflate products were greater for the (Z)-isomers of the iodonium salt precursors indicating that steric effects play a role and implies that these inverted, unrearranged products are derived from in plane (σ*) SN2 reaction. The presence of the remaining, retained, unrearranged enol triflate can be explained by a ligand coupling mechanism (π* SN2) and the fragmentation mechanism(s) do not require the intermediacy of a primary vinyl cation.
 REFERENCE COUNT: 24 THERE ARE 24 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE
 FORMAT

RX(5) OF 10 2 H + 2 O ==> P + Q

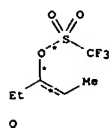
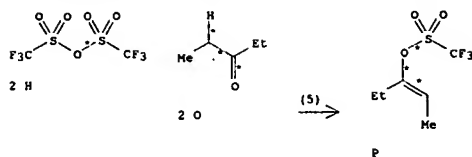
10/518,492



05/05/2006

L2 ANSWER 4 OF 9 CASREACT COPYRIGHT 2006 ACS on STN

(Continued)



RX(5) RCT H 358-23-6, O 96-22-0

STAGE(1)
RGT L 585-46-8 2,6-Di-t-Bu-pyridine
SOL 75-09-2 CH₂Cl₂
CON 12 hours, room temperature

STAGE(2)
SOL 109-66-0 Pentane

PRO P 52149-31-2, Q 52149-30-1
NTE stereoselective

experiment
P-5608

L2 ANSWER 5 OF 9 CASREACT COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 133:257018 CASREACT

TITLE: One-Carbon Homologation of Carboxylic Acids via BtCH₂TMS: A Safe Alternative to the Arndt-Eistert Reaction

AUTHOR(S): Katritzky, Alan R.; Zhang, Suoming; Mostafa Hussein, Abdel Haleem; Fang, Yunfeng; Steel, Peter J.
CORPORATE SOURCE: Center for Heterocyclic Compounds Department of Chemistry, University of Florida, Gainesville, FL, 32611-7200, USA

SOURCE: 5606-5612

CODEN: JOCEAH; ISSN: 0022-3263

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Carboxylic acids are converted into the corresponding homologated acids or

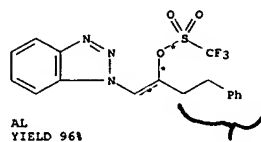
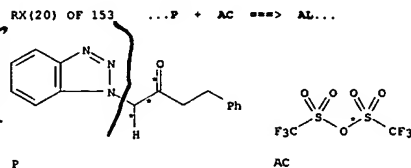
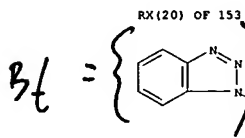
esters, using easily available 1-(trimethyl)silylmethylbenzotriazole as a one-carbon synthon. The effectiveness of the reaction has been investigated on six aryl and seven alkyl carboxylic acids.

REFERENCE COUNT: 39 THERE ARE 39 CITED REFERENCES AVAILABLE FOR THIS

FORMAT

RECORD. ALL CITATIONS AVAILABLE IN THE RE

Table 1,
page 5607



RX(20) RCT P 361379-11-5, AC 358-23-6
RGT AE 108-48-5 2,6-Lutidine

ex (g) Table 1

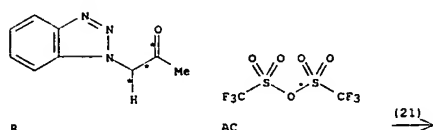


L2 ANSWER 5 OF 9 CASREACT COPYRIGHT 2006 ACS on STN

(Continued)

PRO AL 361379-20-6
SOL 75-09-2 CH₂Cl₂
NTE stereoselective

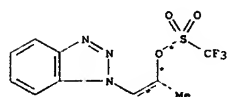
RX(21) OF 153 ...R + AC ==> AN...



R

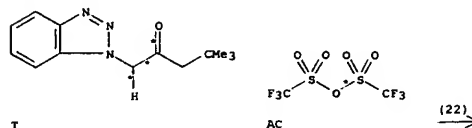
AC

(21)

AN
YIELD 88%

RX(21) RCT R 64882-50-4, AC 358-23-6
RGT AE 108-48-5 2,6-Lutidine
PRO AN 361379-21-7
SOL 75-09-2 CH₂Cl₂
NTE stereoselective

RX(22) OF 153 ...T + AC ==> AP...



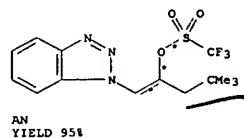
T

AC

(22)

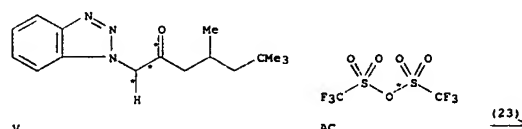
L2 ANSWER 5 OF 9 CASREACT COPYRIGHT 2006 ACS on STN

(Continued)



RX(22) RCT T 314765-22-5, AC 358-23-6
RGT AE 108-48-5 2,6-Lutidine
PRO AN 361379-22-8
SOL 75-09-2 CH₂Cl₂
NTE stereoselective

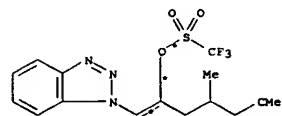
RX(23) OF 153 ...V + AC ==> AO...



V

AC

(23)

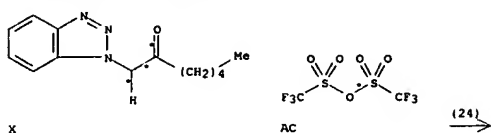
AO
YIELD 98%

RX(23) RCT V 361379-13-7, AC 358-23-6
RGT AE 108-48-5 2,6-Lutidine
PRO AO 361379-23-9
SOL 75-09-2 CH₂Cl₂
NTE stereoselective

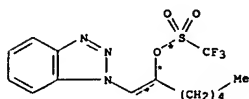
RX(24) OF 153 ...X + AC ==> AP...

ex (j)

L2 ANSWER 5 OF 9 CASREACT COPYRIGHT 2006 ACS on STN (Continued)

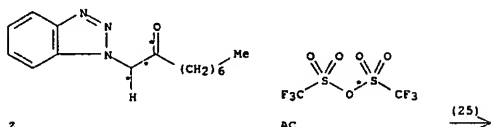


X

AP
YIELD 94%

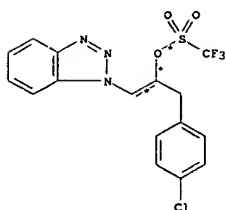
RX(24) RCT X 189343-44-0, AC 358-23-6
RGT AE 108-48-5 2,6-Lutidine
PRO AP 361379-24-0
SOL 75-09-2 CH2Cl2
NTE stereoselective

RX(25) OF 153 ...E + AC ==> AQ...



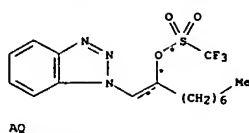
Z

L2 ANSWER 5 OF 9 CASREACT COPYRIGHT 2006 ACS on STN (Continued)

AR
YIELD 82%

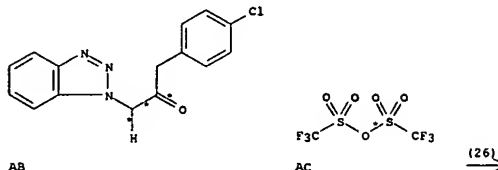
RX(26) RCT AB 306990-72-7, AC 358-23-6
RGT AE 108-48-5 2,6-Lutidine
PRO AR 361379-26-2
SOL 75-09-2 CH2Cl2
NTE stereoselective

L2 ANSWER 5 OF 9 CASREACT COPYRIGHT 2006 ACS on STN (Continued)

AQ
YIELD 90%

RX(25) RCT Z 304459-92-5, AC 358-23-6
RGT AE 108-48-5 2,6-Lutidine
PRO AQ 361379-25-1
SOL 75-09-2 CH2Cl2
NTE stereoselective

RX(26) OF 153 ...AB + AC ==> AR



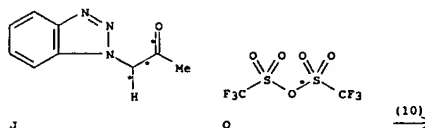
AB

AC

(26)

L2 ANSWER 6 OF 9 CASREACT COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 134:71356 CASREACT
TITLE: BtCH2TMS-Assisted Homologation of Carboxylic Acids: A
Safe Alternative to the Arndt-Eistert Reaction
AUTHOR(S): Katritzky, Alan R.; Zhang, Suoming; Fang, Yunfeng
CORPORATE SOURCE: Center for Heterocyclic Compounds Department of
Chemistry, University of Florida, Gainesville, FL,
32611-7200, USA
SOURCE: Organic Letters (2000), 2 (24), 3789-3791
CODEN: ORLEF7; ISSN: 1523-7060
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
AB One-carbon homologation of carboxylic acids is achieved by (i) treatment
of an acyl chloride with
1-[(trimethylsilyl)methyl]-1H-1,2,3-benzotriazole
(BtCH2TMS) to afford N-(acylmethyl)benzotriazoles, followed by (ii)
conversion with triflic anhydride into RC(OTf):CHBr, and (iii) the
subsequent reaction with NaOCH3 followed by 1N HCl to afford esters
RCH2CO2R' in overall yields of 50-70%. For the aliphatic compds.,
treatment
with p-toluenesulfonic acid followed by TBAF/THF afforded acids RCH2COOH.
REFERENCE COUNT: 14 THERE ARE 14 CITED REFERENCES AVAILABLE FOR
THIS
FORMAT RECORD. ALL CITATIONS AVAILABLE IN THE RE

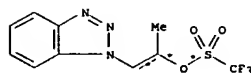
RX(10) OF 69 ...J + O ==> V...



J

O

(10)

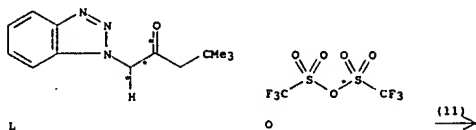
V
YIELD 88%

RX(10) RCT J 64882-50-4, O 358-23-6
STAGE(1)
RGT Q 108-48-5 2,6-Lutidine
SOL 75-09-2 CH2Cl2

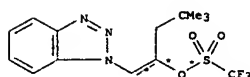
L2 ANSWER 6 OF 9 CASREACT COPYRIGHT 2006 ACS on STN (Continued)
STAGE(2)
SOL 110-54-3 Hexane

PRO V 314765-31-6

RX(11) OF 69 ...L + O ==> W...



L



W
YIELD 95%

RX(11) RCT L 314765-22-5, O 358-23-6

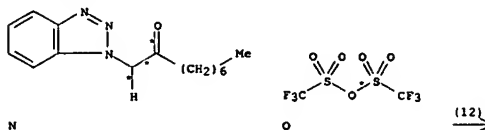
STAGE(1)
RGT Q 108-48-5 2,6-Lutidine
SOL 75-09-2 CH2Cl2

STAGE(2)
SOL 110-54-3 Hexane

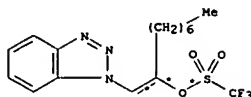
PRO W 314765-33-8

RX(12) OF 69 ...N + O ==> X...

L2 ANSWER 6 OF 9 CASREACT COPYRIGHT 2006 ACS on STN (Continued)



N



X
YIELD 90%

RX(12) RCT N 304459-92-5, O 358-23-6

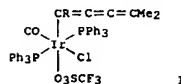
STAGE(1)
RGT Q 108-48-5 2,6-Lutidine
SOL 75-09-2 CH2Cl2

STAGE(2)
SOL 110-54-3 Hexane

PRO X 314765-35-0

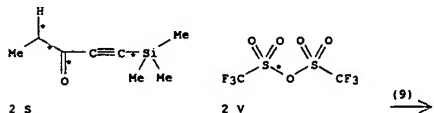
L2 ANSWER 7 OF 9 CASREACT COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 106:138608 CASREACT
TITLE: Kinetics, stereochemistry, and mechanism of interaction of Vaska's complex with ethynylvinyl triflates. Formation of novel σ -butatrienyliridium compounds
AUTHOR(S): Stang, Peter J.; Dixit, Vandana; Schiavelli, Melvyn D.; Drees, Paul
CORPORATE SOURCE: Dep. Chem., Univ. Utah, Salt Lake City, UT, 84112, USA
SOURCE: Journal of the American Chemical Society (1987), 109(4), 1150-6
CODEN: JACSAT; ISSN: 0002-7863
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



AB The reaction of Vaska's complex $[(\text{Ph}_3\text{P})_2\text{Ir}(\text{CO})(\text{Cl})]$ with $\text{Me}_2\text{C}=\text{C}(\text{O}_3\text{SCF}_3)\text{C}\equiv\text{C}\text{bond.CR}$ ($\text{R} = \text{H}, \text{D}, \text{Me}, \text{Ph}, \text{SiMe}_3$) was investigated. Oxidative addition readily occurs in benzene or toluene at room temperature to give hexacoordinate $\text{Ir}(\text{III})$ butatrienyl complexes I ($\text{R} = \text{same}$). Rate studies indicate steric inhibition by bulky substituents on the terminal acetylenic C and give high neg. entropies of activation. The reaction occurs with complete (or nearly complete) retention of olefin stereochem. A two-step $\text{S}_\text{N}2$ process with syn approach of the incoming Ir nucleophile is proposed to account for these observations.

RX(9) OF 28 ...2 S + 2 V ==> M + P...

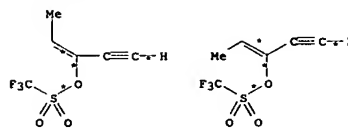


2 S

2 V

(9)

L2 ANSWER 7 OF 9 CASREACT COPYRIGHT 2006 ACS on STN (Continued)



M

YIELD 77% (45)

P

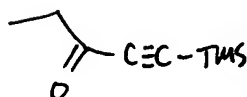
YIELD 77% (75)

RX(9) RCT S 18387-58-1, V 358-23-6
RGT W 38222-83-2 Me-(t-Bu)2-pyridine
PRO M 106211-71-6, P 106211-72-7
SOL 75-09-2 CH2Cl2



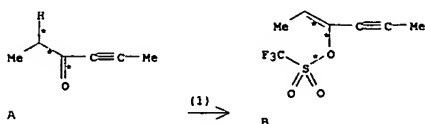
references Synthesis, 1979, 438
(Stang et al.)

Synthesis, 1982, 85 (IDS)



L2 ANSWER 8 OF 9 CASREACT COPYRIGHT 2006 ACS on STN
 ACCESSION NUMBER: 104:148249 CASREACT
 TITLE: The preparation of unsymmetrical diacetylenes from alkenynyl triflates
 AUTHOR(S): Stang, Peter J.; Dixit, Vandana
 CORPORATE SOURCE: Chem. Dep., Univ. Utah, Salt Lake City, UT, 84112, USA
 SOURCE: Synthesis (1985), (10), 962-3
 CODEN: SYNTBF; ISSN: 0039-7881
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 AB RC.tplbond.CC(O3SCF3):CHMe (I; R = Me, Ph) were converted in 85% yield to RC.tplbond.CC.tplbond.CMe by treatment with 2,6-(Me3C)2C6H3OK in glyme. Me3SiC.tplbond.CC.tplbond.CMe was similarly prepared in 45% yield by treating I (R = Me3Si) with (Me2CH)2NLi in glyme. I were prepared by treating RC.tplbond.CCOCH2Me with (CF3SO2)2O in the presence of 2,6-di-tert-butyl-4-methylpyridine.

RX(1) OF 9 A ==> B...



RX(1) RCT A 10575-41-4
 RGT C 38222-83-2 Me-(t-Bu)2-pyridine, D 358-23-6
 (F3CSO2)2O
 PRO B 101160-51-4
 SOL 75-09-2 CH2Cl2

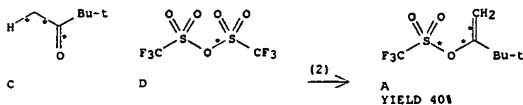
RX(2) OF 9 F ==> G...



RX(2) RCT F 19307-74-5
 RGT C 38222-83-2 Me-(t-Bu)2-pyridine, D 358-23-6

L2 ANSWER 9 OF 9 CASREACT COPYRIGHT 2006 ACS on STN
 ACCESSION NUMBER: 80:82004 CASREACT
 TITLE: Vinyl triflates in synthesis. I.
 AUTHOR(S): Hargrove, Robert J.; Stang, Peter J.
 CORPORATE SOURCE: Chem. Dep., Univ. Utah, Salt Lake City, UT, USA
 SOURCE: Journal of Organic Chemistry (1974), 39(4), 581-2
 CODEN: JOCEAH; ISSN: 0022-3263
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 AB The elimination of CF3SO3H from Me3CC(O3SCF3):CH2 (I) to give MeCC.tplbond.CH is catalyzed by pyridine. Pinacolone reacts with (CF3SO2)2O to give I.

RX(2) OF 3 C + D ==> A...



RX(2) RCT C 75-97-8, D 358-23-6
 RGT E 110-86-1 Pyridine
 PRO A 27701-32-2
 SOL 56-23-5 CCl4
 NTE Classification: Isomerisation; O-Sulphonation; # Conditions: triflic anhydride; CCl4 pyridine; 15 deg 60h

soln of
 (c)
 0.02 mol
 + pyridine
 0.022 mol

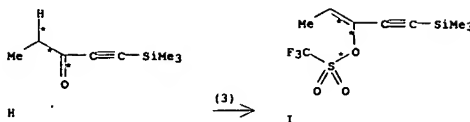


-22°C
 15 min then warm to 15°C for 60 hr.

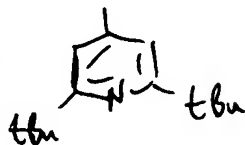
add in TF_2O (0.022 mol)

L2 ANSWER 8 OF 9 CASREACT COPYRIGHT 2006 ACS on STN (Continued)
 (F3CSO2)2O
 PRO G 101160-52-5
 SOL 75-09-2 CH2Cl2

RX(3) OF 9 H ==> I...



RX(3) RCT H 18387-58-1
 RGT C 38222-83-2 Me-(t-Bu)2-pyridine, D 358-23-6
 (F3CSO2)2O
 PRO I 101160-53-6
 SOL 75-09-2 CH2Cl2



methods in Stang et al.

Synthesis 1979, 438

references - Dueber et al. Angew. Chem
 Int. Ed. Engl. 9, 521 (1970)

1D) { Stang & Dueber, Org. Syn.
 54, 79 (1974)